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### **A New Electronic Transition in SeO**

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## A NEW ELECTRONIC TRANSITION IN SeO

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ABSTRACT

A new electronic band-system in emission has been recorded in the region  $6150\text{--}5250\text{ \AA}^{\circ}$  using a transformer discharge through flowing  $\text{SeO}_2$  vapor. Twentyfour weak red degraded bands have been observed and are attributed to the molecule  $\text{SeO}$ . A vibrational analysis of the observed bands leads to the conclusion that the upper state involved in the transition is new state b which is situated at  $17338.5\text{ cm}^{-1}$  above the ground state. The lower state involved in the transition is the ground state of the molecule. The values of  $\omega_e$  and  $\omega_e x_e$  for the upper and lower states are found to be :

$$\text{Upper State b : } \omega_e = 885.2\text{ cm}^{-1}, \quad \omega_e x_e = 5.85\text{ cm}^{-1}$$

$$\text{Lower State X : } \omega_e = 914.8\text{ cm}^{-1}, \quad \omega_e x_e = 4.87\text{ cm}^{-1}$$

INTRODUCTION

The electronic band-system of  $\text{SeO}$  has been investigated by Asundi et al (1), Choong (2), and Barrow et al (3). Only one band-system involving the ground state X and the upper state A has been known so far. According to the work of Barrow et al (3) the upper and the lower states involved in the transition  $A \rightarrow X$  are both  $3\Sigma^-$ .

A literature survey of the electronic band-system of the monoxides of group VIA elements reveals that in  $\text{TeO}$ ,  $\text{O}_2$  and  $\text{SO}$  more than one electronic band-system has been known. In the molecule  $\text{NBr}$  (4) which is isoelectronic with  $\text{SeO}$ , a band-system has been known in the region  $6400\text{--}5650 \text{ \AA}^\circ$ . The present investigation was undertaken with a view to discover new electronic transitions in  $\text{SeO}$ , and a new band-system in the region ( $6150\text{--}5250 \text{ \AA}^\circ$ ) has been recorded in addition to the known A - X system. From our studies we have concluded that this new electronic transition involve the ground state X and a new upper electronic state which we have labeled as the b-state.

### EXPERIMENTAL

The emission spectrum of  $\text{SeO}$  was recorded by exciting a pure sample of  $\text{SeO}_2$  under flowing condition in a conventional  $\pi$ -type discharge tube using a power transformer. The chemical was 99.9% pure and was obtained from May and Backer Ltd., London. The band-spectra were recorded on Ilford-HP3 hyper sensitive panchromatic plates on a Steinheil 3-prism glass spectrograph which has a reciprocal linear dispersion of about  $3 \text{ \AA}^\circ/\text{mm.}$  at  $4400 \text{ \AA}^\circ$ . The exposure time and slit width were 3-hours and 20 microns respectively. The intensity of the recorded bands was found to be very weak (too weak to be reproduced in a journal). The observed bands were measured on a Russian made Comparator (Model No. EZA-2) using iron lines as reference. The band heads of the more intense bands were measured with a precision of  $\pm 2 \text{ cm}^{-1}$ . The weaker bands were measured with a precision of  $\pm 4 \text{ cm}^{-1}$  by making pinholes at the position of their band heads.

RESULTS AND DISCUSSIONA : The known A-X system:

Excitation of the  $\text{SeO}_2$  in the discharge tube gave rise to the known A-X system of SeO. Ten strong bands of this system were measured and their wavelengths were found to agree with those reported by Pearse and Gaydon (5).

B: The New Band-System :

Twentyfour weak bands, degraded to the red were observed in the region 6150-5130  $\text{\AA}$ . The wavelength, wavenumber, and the vibrational assignment of the bands are entered in Table I. The bands fit very nicely into the Deslandres' scheme of a diatomic molecule as shown in Table II. The molecular constants obtained from the vibrational analysis have been entered in Table III.

The value of the  $\omega_e$  for the lower state has been found to be  $914.8 \text{ cm}^{-1}$  which agrees very well with the ground state frequency of  $914.69 \text{ cm}^{-1}$  reported by Barrow et al (3), giving a very strong evidence that the lower state involved in the transition of this new system is the  $X^3\Sigma^-$  state of SeO.

The value of  $\omega_e$  for the upper state has been found to be  $895.2 \text{ cm}^{-1}$ . On the basis of our experimental data it is not possible to arrive at any conclusion regarding the nature of this upper electronic state of the molecule which we have labeled as b-state. However, we observe that in  $\text{O}_2$  (6) and in SO (7) a low-lying  $b^1\Sigma^+$  state has been found<sup>and</sup> a forbidden transition  $b^1\Sigma^+ - X^3\Sigma^-$  has also been observed. The values of  $\omega_e'$ ,  $\omega_e''$  and the ratio  $\omega_e'/\omega_e''$  for the  $b^1\Sigma^+$  and  $X^3\Sigma^-$  states in  $\text{O}_2$  and SO have been given in Table IV, and

TABLE I

Wavelengths, Wavenumbers, and the Vibrational  
Assignment of the New Bands of SeO

S.No.	Wavelengths in Å	Wavenumbers (vacuum) in cm <sup>-1</sup>	Assignment (v', v'')
1	6139.1	16284	(6,7)
2	6117.3	16343	(4,5)
3	6106.6	16371	(3,4)
4	6095.4	16401	(2,3)
5	6088.3	16420	(1,2)
6	6079.5	16444	(0,1)
7	5835.9	17130	(6,6)
8	5821.7	17172	(5,5)
9	5809.5	17208	(4,4)
10	5796.1	17248	(3,3)
11	5784.0	17284	(2,2)
12	5773.0	17317	(1,1)
13	5762.4	17349	(0,0)
14	5574.7	17933	(7,6)
15	5558.6	17985	(6,5)
16	5543.1	18035	(5,4)
17	5528.8	18082	(4,3)
18	5513.2	18133	(3,2)
19	5499.8	18177	(2,1)
20	5486.0	18223	(1,0)
21	5287.8	18906	(5,3)
22	5271.3	18965	(4,2)
23	5254.2	19027	(3,1)
24	5239.3	19081	(2,0)

TABLE II

Deslandres' Scheme for the New Bands of SeO

$v'$	$v''$	0	1	2	3	4	5	6	7
0		17349	905	16444					
		874		873					
1		18223	906	17317	897	16420			
		858		860		864			
2		19061	904	18177	893	17284	883	16401	
				850		849		847	
3			19027	894	18133	885	17248	877	16371
					832		834		837
4					18965	883	18082	874	17208
							824	827	829
5						18906	871	18035	863
								813	
6								17985	855
									17130
									846
									16284
									803
7									17933

we find that the molecule SeO fits into the trend nicely. This observation together with the fact that the intensity of the bands of this new system is quite weak leads to the suggestion that the transition involved is probably  $b^1\Sigma^+ \rightarrow X^3\Sigma^-$ . Of course, the rotational structure of the bands must be resolved and studied before arriving at any definite conclusion regarding the nature of the upper electronic state.

TABLE III

Molecular Constants for the b and X States of SeO

State	$\omega_e(\text{cm}^{-1})$	$\omega_e(\text{cm}^{-1})$	$\omega_{ex}(\text{cm}^{-1})$
b	17338.5	885.2	5.85
X	0	914.8	4.87

TABLE IV

 $\omega_e'$ ,  $\omega_e''$  and  $\omega_e'/\omega_e''$  in the b and X States of O<sub>2</sub>, SO and SeO

Molecule	$\omega_e'(\text{cm}^{-1})$	$\omega_e''(\text{cm}^{-1})$	$\frac{\omega_e'}{\omega_e''}$	Ref.	Electronic Transition	Wavelength region Å°
O <sub>2</sub>	1432.68	1580.36	0.91	6	$b^1\Sigma^+ - X^3\Sigma^-$	(5380-8803)
SO	1068.66	1149.22	0.94	7	$b^1\Sigma^+ - X^3\Sigma^-$	(9600-10500)
SeO	885.2	914.8	0.95	Present work	$b^1\Sigma - X^3\Sigma^-$	(5250-6150)

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